HARECES Measurements on Hexagonal Boron Nitride

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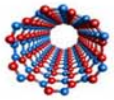
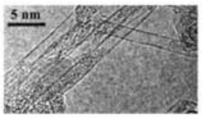




High resolution TEM image of a boron nitride nanotube

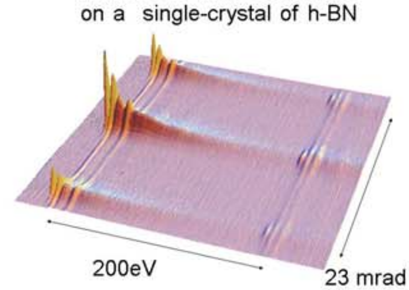
Motivation

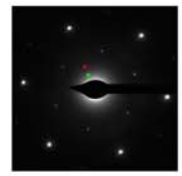
Hexagonal boron nitride (**h-BN**) is an insulating, anisotropic material structurally analogous to semimetallic graphite. Recently the interest of h-BN has increased due to the development of synthesis procedures for creating boron nitride nanotubes (**BNNTs**), which form as h-BN sheets rolled up into a cylindrical shape.

In the specific case of an anisotropic crystal like h-BN, the use of electron energy loss spectroscopy (EELS) in a transmission electron microscope allows us to probe this anisotropy in the electronic structure through the use of angle-resolved spectroscopy.

In this work we are studying the electronic and dielectric properties of h-BN by measuring angle-resolved EELS (core loss and low loss regions) in the Tecnai F-20 electron microscope using high angular resolution electron channeling electron spectroscopy (**HARECES**).

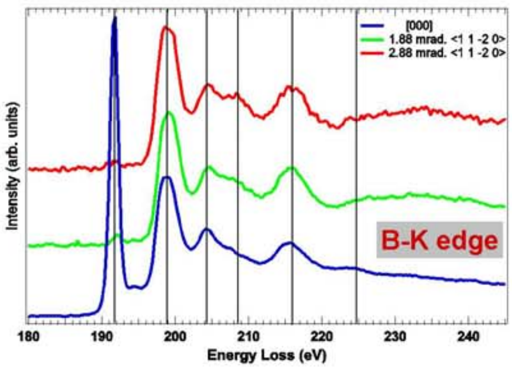
HARECES measurements on a single-crystal of h-BN

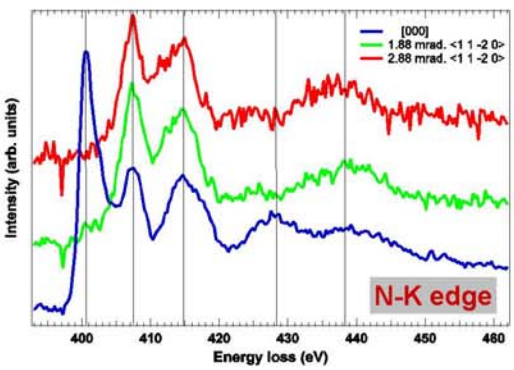




Selected area electron diffraction of a single-crystal of h-BN. Circles: scattering vectors

Results





Core loss spectra

B-K edge

- The prominent, narrow and intense peak at 191.8 eV corresponds to the B 1s - π^* resonance, which is associated with sp^2 hybridization and planar bonding. This peak disappears if the momentum transfer ***q*** is perpendicular to the *c*-axis, showing that it is entirely due to $2p_z$ orbitals.
- The $\sigma*$ peak at 198 eV is mostly due to 2s and $2p_{x,y}$ orbitals.
- Further smaller peaks at higher energy losses can be correlated with transitions into 3s and 3p orbitals.

N-K edge

- The two main peaks at 402 and 409 eV, which are similarly related to N $2p_z$ and $2p_{x,y}$ orbitals, as in the case of the B-K edge.

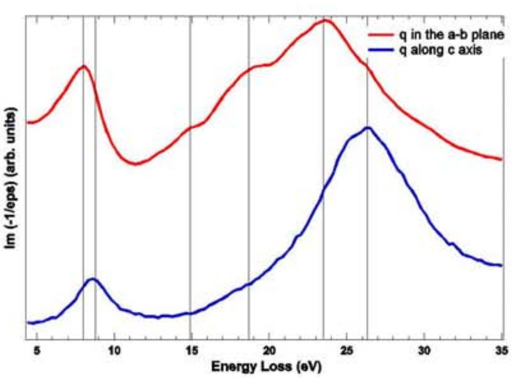
Low loss spectra

In plane orientation:

- Only the transitions π to π^* and σ to $\sigma*$ are allowed.
- The loss function in this orientation is dominated by the π and total $(\pi + \sigma)$ plasmons at 8.6 and 26.2 eV respectively.

Out of plane:

- The peaks at 7.7 and 23 eV correspond to the plasmons or collective excitations.
- The other peaks correspond to interband transitions.



Impact

We have acquired resolved angle-resolved EELS (**core loss** and **low loss** regions) on a single-crystal of h-BN. These results significantly improve on the older work and they show that HARECES is the most powerful technique to perform momentum resolved EELS.

Future directions

Initially our work is concentrating on understanding the observed changes in the electronic structure of small single crystal specimens. Once completed, we will be applying these interpretations to results obtained from boron nitride nanotubes.

Particularly, we will focus in the study of the low loss spectra because this information is very important to enable a better understanding of the band structure of this material. There exists in the scientific community a controversy between the nature and value of the energy band gap.

R. Arenal, M. Kociak, and N.J. Zaluzec (in preparation)

ARGONNE NATIONAL LABORATORY

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